Chemistry in aqueous solutions as described by ab initio molecular dynamics: case of a green catalyst under “in-water” and “on-water” conditions

Rodolphe Pollet[a], Himansu Biswal[b]

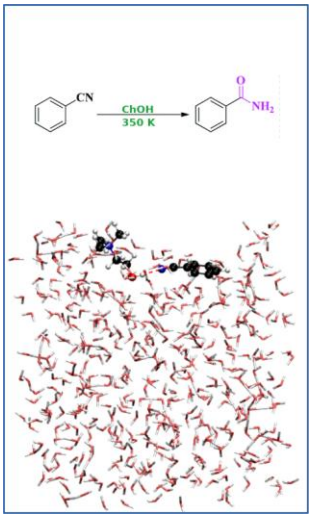
[a]*Université Paris-Saclay, CEA, CNRS, NIMBE*

[b]*School of Chemical Sciences, National Institute of Science Education and Research (NISER)*

rodolphe.pollet@cea.fr

Ab initio molecular dynamics (AIMD) is a valuable tool for the investigation of chemical reactions involving the formation or breaking of covalent bonds as well as subtle interactions between solute and solvent molecules or ions. The computational cost that precluded the study of large systems or long-time properties has been recently reduced thanks to more efficient algorithms and new strategies of code parallelization [1].

We will focus on the theoretical study of an environmentally benign catalyst, namely choline hydroxide (ChOH), for the conversion from nitriles to amides [2], with water as a solvent, under two specific conditions: “in-water” (or bulk) conditions and “on-water” (at the air-water interface) conditions [3]. This investigation emphasizes some characteristics of aqueous solutions, namely the importance of the dynamics of hydrogen bonds, the possible occurrence of isomeric conversions, the structural diffusion of the hydroxide anion, and the influence of interfacial conditions.



References

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